MATHEMATICAL MODELS AND ALGORITHMS FOR THE COMPUTER PROGRAM 'WOLF'

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THE COMPUTER PROGRAM 'WOLF'

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1. Introduction

The computer program FLOW finds the non-relativistic self-consistent set of two-dimensional ion trajectories and electric fields (including space charges from ions and electrons) for a given set of initial and boundary conditions for the particles and fields. The combination of FLOW with the optimization code PISA (ref. 1) gives the program WOLF that finds the shape of the emitter that is consistent with the plasma forming it, and in addition varies physical characteristics such as electrode-positions, -shapes, and -potentials so that some performance characteristics are optimized. The motivation for developing these programs was the desire to design optimum ion source extractor/accelerator systems in a systematic fashion (ref. 2). The work on the programs started in the spring of 1973 and was a team effort by William S. Cooper, Klaus Halbach, and Steven B. Magyary, with the responsibilities distributed as follows: W.S.C., as the "customer" and user, specified in essence what the program should do, and provided the information and understanding relating to the plasma-determined boundary conditions of the emitter; K.H. formulated the mathematical models and, where necessary, algorithms; and S.B.M. translated that into a usable fast com-

puter program. As is true for every good team, each member also made contributions to the parts of the effort that were not his direct responsibility.

It is the purpose of this report to explain and derive the mathematical models and algorithms that approximate the real physical processes. Serving (mostly) to document a computer program, it has been attempted to make this report as self-contained as possible by including as many relevant topics as could be done without making the report unwieldy. Even basically "text book" subjects have been included when it was considered not likely that all potential readers would have the necessary familiarity with them. The material described goes a little bit beyond the present status of FLOW by replacing some of the originally used algorithms with newer ones that are now being incorporated into the program, or will be incorporated in the immediate future. Since the computer program was developed under time pressure, because of the desire to produce results very fast, and also because of competition with other work, there may be some parts that are not quite as elegant or as fast as one could make them. While it is unlikely that this led to significant waste of computer time, suggestions for improvements would be greatly appreciated, particularly since further development of the program is an ongoing process.

To make a simple updating of this report at a later time possible, and also to improve its readability, all detailed mathematical developments have been put into appendices, and an attempt has been made to make the report understandable without having to read the appendices. Consequently, the appendices have been formulated in such a way that each is an essentially self-contained chapter, with only few references to other appendices.

2. Units and Notation

Since the physical dimensions of the structures to be modeled are of the order of centimeters, and not meters, we don't use S.I. units, but Volt, Amperes, Seconds and Centimeters.

We use an x-y coordinate system to describe the two-dimensional geometry we are dealing with. It is frequently convenient to use complex arithmetic, and we then use $z = x + iy$, indicate real and imaginary parts of complex numbers by Re and Im, and indicate the complex conjugate of a number by *. While the variable names in the computer programs often are the same as the ones used here, this is not always so. It would also have been inconvenient to always have the same quantity associated with every symbol used in the appendices. While this can hardly lead to misunderstandings, there is one exception: The symbol V describes the scalar potential everywhere with the exception of Appendix F, where it describes the negative of the scalar potential.

In the appendices it is repeatedly necessary to perform cyclical sums over quantities that are associated with the corners of triangles. When such summations go over the three corners of a triangle, the sum is written by writing down one specific term, preceeded by $\sum_3$. Similarly, we write $\sum_6$ for cyclical sums that go over all six points surrounding a mesh point. In some, but not all, cases it is important that the three corners of a triangle are sequenced in proper cyclical order, namely going in counterclockwise direction around the triangle. In the context of reviewing some surface integral formulas, Appendix D gives two explicit formulas for the area of a triangle that are used frequently in Appendices A and C and can also be used to determine correct cyclical order. The derivation of these formulas involves some manipulation of cyclical sums that is also often used.

3. The Program FLOW

    a. General Remarks

This program accomplishes the objective stated in the Introduction in the following way: The two-dimensional space that one wants to treat is covered by an irregular triangular mesh (Section 3b), with boundary sections being either on given scalar potentials, or on electric field lines. The program POISSON (Section 3b) calculates the scalar potential at the mesh points.

It is assumed that the electrons in the plasma in the vicinity of the ion emitter surface have a Boltzmann distribution with temperature $T_e = eV_e/k$, and that, as a consequence, the electron density in the region of interest is proportional to exp (scalar potential/V_e). The subroutine ELECTR deposits charges at the mesh points that represent the space charge caused by these Boltzmann electrons.

Ions coming from the emitter will have various charge to mass ratios and will have a spread in energy and emission angle. This physical reality is modeled by letting a number of beams emerge from each line element that represents a part of an emitter surface. Each such beamlet is characterized by a charge to mass ratio, the current it represents, and an initial energy and trajectory direction. The routine BTRACE traces each beamlet and deposits the appropriate charges at mesh points. The trajectory calculation does not take into account relativistic effects, and the self-produced magnetic field is consequently also ignored.

    b. POISSON

The reasons for using this program (originally developed by A. Winslow, ref. 3) to solve the electrostatic field problem are manyfold:

The difference equations are solved in an irregular triangular mesh that is produced by a mesh generator that is part of the POISSON program package. This makes it possible to have a large density of mesh points where one needs it, and also has the advantage of having all surfaces, like emitters, electrodes, and field lines that are a boundary, defined by mesh lines, without having to resort to interpolation. This in turn leads to comparatively simple difference equations. They are derived in Appendix A mainly to show how the space charges have to be treated: The space charge distribution in the mathematical model used here consists of many curved line charges and the charges resulting from the electrons, i.e., is extremely nonuniform. The fact that the equivalent space charges have to be distributed among the corners of every triangle in such a way that their "center of mass" is the same as that of the distribution they represent is quite plausible, but not so trivial as to make a derivation and proof unnecessary. With given space charges, the program solves for the scalar potential values at the mesh points with an overrelaxation method that finds its own optimum over-relaxation factor, and terminates the iteration process when a convergence criterion indicates that one is sufficiently close to the solution. The program was originally written to find the vector potentials A from which one derives magnetic fields $\vec{B}$. Except for removing sections of the magnetic code that are not needed for this application, no changes were made, and the variable names (vector potential A, etc.) reflect that.

c. ELECTR

Since the density of the Boltzmann electrons is proportional to exp (scalar potential/V_e), they are usually ignored beyond some distance

from the emitter. In the region where they are considered, they are taken into account by calculating for every triangle the total charge and its "center of mass". From that, the charges are calculated for each corner of the triangle, and are used with the appropriate underrelaxation factor (see Section 3e), to update the electron charge array. The relevant formulas are derived in Appendix C and summarized at the end of Appendix C.

d. BTRACE

Each beamlet, endowed with a charge to mass ratio and a current, is traced through one triangle at a time, starting with given initial energy and trajectory direction at the emitter. After having determined the trace through a particular triangle, the charge, and its "center of mass", are calculated, and then the proper charges for the three corners of the triangle are computed and used to update the corresponding array. The relevant formulas are derived in Appendix J, both with and without a uniform magnetic field perpendicular to the x-y-plane.

e. Sequencing of Subroutine Calls in FLOW

Every time after POISSON has calculated new scalar potentials at the mesh points, ELECTR is called to recalculate the electron charge deposition. To avoid computational instabilities and speed up convergence, the newly calculated electron charges are not deposited directly as calculated, but compared with the previously existing electron charges. The recommended change is not fully applied, but first multiplied with an underrelaxation factor that lies between .05 and .3. After having alternated between POISSON and ELECTR a sufficient number of times, the recommended changes in electron charge become small enough that one can calculate the beam traces and deposit the thus generated ion charges. Then the POISSON-ELECTR

iteration starts again until it has converged, giving the signal to use BTRACE again. This process is repeated until the ion charge-changes are sufficiently small to indicate convergence of the FLOW evaluation. It is the opinion of all involved persons that this sequencing and underrelaxation scheme is, although it works, at present the weakest part of the program. Past "experimentation" has led to the belief that substantial improvements may be possible, but are not going to be easily obtained. It should also be pointed out in this context that some well posed evaluation problems have been encountered (for instance when in some region the majority of ions is reflected by suitably applied potentials) where convergence was extremely slow, or convergence could not be achieved at all.

f. Test Problem

For computer programs of the nature and complexity of FLOW it is very desirable to have test problems that are non-trivial for the computer, yet have analytical solutions. The reason for wanting such test problems is not only the need for finding possible "bugs", but also to see what the discretization-consequences are. Such a study can, for instance, indicate what types of mesh symmetries are preferable, or should be avoided.

The "cut off" one-dimensional diodes with matching Pierce-type electrodes represent a family of test problems that is very well suited for our purposes, and they are discussed in some detail in Appendix F. The only important feature of the general case that cannot be treated is the angular distribution of the ions leaving the emitter. That is clearly not a significant shortcoming, since a test with all ions being emitted perpendicularly to the emitter is probably more severe (because of possible mesh-geometry-influence) than one with some angular distribution.

Equations (F-15) and (F-16) give an analytical expression for the matching electrode structure of the general "cut off" one-dimensional diode, and requires straightforward numerical integration for actual application. Equation (F-19) describes a special class of these diodes that allows representation of the integral in closed form. That formula was used for one case of no electrons, and only one ion species, with non-zero initial energy, and $V_o' = 0$, to construct a test problem before electrons were introduced, and Fig. (F1), (F2) show the result of such a test run: Fig. (F1) shows the vacuum-equipotentials, and the trajectories of the ions in the vacuum fields. After the iteration process between POISSON and BTRACE converged, Fig. (F2) was plotted, showing precisely the expected equipotential- and trajectory-shapes.

4. The Program WOLF

The FLOW calculations all by themselves are not realistic, since one does not know what the shape of the emitter surface should be. By making certain assumptions about the nature of the plasma behind the emitter surface (ref. 2), one can define this shape by requiring that everywhere on the emitter the electric field has a value that is related to the initial conditions and other properties that are associated with the ions and electrons (see Appendix H). It is furthermore desirable to optimize some properties of the beams at the output end of an extractor structure. The quantities considered exclusively so far are the angles θ between the tangents to the trajectories at the exit, and a given direction. Both the constancy of the electric field along the emitter surface and the parallelity of the exiting ions are approximately obtained by minimizing the function

$$\sum_i W_i (E_i - E_o)^2 + \sum_k W_k (\theta_k - \theta_o)^2 \ ,$$

with appropriately chosen weights W_i, W_k. It is fairly easy to add to this function, or to make the prescribed values of the electric field or exit direction (assumed constant (E_o, θ_o) above) dependent on the beam. The parameters used for optimization are the shape of the emitter surface, positions, shapes, and potentials of electrodes, and possibly also some properties associated with the emitter forming plasma. The optimization is accomplished by linking FLOW with the optimization program PISA (ref. 1), a least squares optimization program that obtains rapid convergence by controlling the size of the parameter changes with a self-adjusting under-relaxation method.

5. Future Development

The program package described in this report was developed to model two dimensional structures. It would be fairly easy to modify the affected programs to describe problems with cylindrical symmetry, provided one does not want to deal with skew ion trajectories. Incorporating trajectories that do not stay in a meridional phase adds not only a new dimension to the initial conditions, but requires also development of an additional trajectory tracing code.

Lifting the restriction to non-relativistic particles requires calculation of the self-magnetic field, and a new algorithm for the trajectory computation. Both of these modifications would require some work, but should not be too difficult to implement.

Acknowledgements

W. S. Cooper, S. B. Magyary and A. C. Paul read the first draft of this report and made a large number of suggestions for improving its readability. If this report is successful in that respect, they deserve the credit; if not, I deserve the blame.

APPENDIX A

The Difference Equations for Solving the Two-Dimensional Poisson Equation

In order to approximately solve the Poisson equation

$$\text{div}(\varepsilon \vec{E}) = \rho \ , \tag{A1}$$

with

$$\vec{E} \equiv -\text{grad } V \tag{A2}$$

representing the electric field, V the scalar potential, ε the relative dielectric constant multiplied by $\varepsilon_0 = 8.85 \cdot 10^{-14} \ A \sec V^{-1} cm^{-1}$, and ρ the charge density, we use the variational principle

$$T = \int (\varepsilon E^2 - 2\rho V)da = \text{Min} \ . \tag{A3}$$

This integral is to be taken over the whole problem area, with the desired boundary conditions imposed at the boundaries. While this variational principle is a regular textbook subject, some readers will use it infrequently enough to make it worthwhile to include its proof in Appendix B. The variational principle will be used in both directions, i.e., the fact will be used that if Eq. (A3) is satisfied it follows that (A1) is satisfied, and vice versa.

The values of V are introduced at the mesh points of an irregular triangular mesh (see Fig. A1) that has the property that each mesh point (except those on a boundary of the problem) is a vertex of six triangles. The x,y coordinates of the mesh points are computed by a mesh generator, (ref. A1) with mesh regions defined in such a way that one obtains approximately the desired mesh size in every such region of the problem geometry. ε is assumed to be constant throughout every triangle, but may

have different values in different triangles in the general case; since there
is no extra computation associated with this generalization, we treat ε that
way, even though for the present application ε will have the same value ε_0
throughout the whole problem. There are no restrictions on $\rho(x,y)$.

In order to be able to calculate, and then minimize, the integral in
(A3), one has to make a rule that determines how V is to be calculated
inside every triangle. A rule that leads to the simplest meaningful differ-
ence equation is the following:

The potential inside a triangle is a linear function of the values
of the scalar potential at its vertices, depends in addition only on the
charge density in the triangle, and is invariant to translation and rotation
of the coordinate system.

This rule has the consequence, as will be seen in more detail below,
that when optimizing T (Eq. A3) with respect to the potential at a parti-
cular mesh point, one obtains a linear relationship between that potential
and the potentials of the other vertices of the six triangles surrounding
the point under consideration.

To arrive at a description of V within a triangle, we discuss first
the consequences of a discontinuity of V, as one goes from one triangle to
another across a line connecting two mesh points. Clearly, a singularity
would result for $\vec{E}$, and this singularity would not disappear upon calcula-
ting $\int \varepsilon E^2 da$. To prevent this from happening, V has to vary along a line
connecting two mesh points in a unique way, depending only on the values of
V at these two mesh points. The only reasonable function that will do this
is the linear function of x,y that assumes the proper V-values at the two
mesh points.

Assuming for the moment $\rho = 0$ within a triangle, it is clear that the function V_0 that minimizes the contribution from that triangle to T must satisfy Eq. (A1) with $\rho = 0$ within the triangle. With the above stated boundary condition, V_0 must obviously be a linear function of x and y in the triangle, assuming the values V_1, V_2, V_3 at its vertices. For $\rho \neq 0$, we can set $V = V_0 + V_4$, with V_4 satisfying Eq. (A1) with non-zero ρ, subject to the boundary condition $V_4 = 0$ along the sides of the triangle. With $\vec{E}_0 = -\text{grad } V_0$, $\vec{E}_4 = -\text{grad } V_4$, the contribution to T resulting from the triangle under consideration becomes

$$U = \int [\epsilon (\vec{E}_0 + \vec{E}_4)^2 - 2\rho (V_0 + V_4)] da/2,$$

and its derivative with respect to the potential V_1, at vertex 1 is

$$U_1' = \int \epsilon \vec{E}_0 \frac{\partial \vec{E}_0}{\partial V_1} da - \int \rho \frac{\partial V_0}{\partial V_1} da + \int \epsilon \frac{\partial \vec{E}_0}{\partial V_1} \vec{E}_4 da . \tag{A4}$$

In taking this derivative we have used the fact that V_4 does not depend on V_1. We will now proceed to show that the last integral on the right side of Eq. (A4) is zero, meaning that it is sufficient to assume that the potential within a triangle is a linear function of x and y. We then calculate $\partial V_0/\partial V_1$ (Eq. (A7)), and then the first integral on the right side of Eq. (A4), (Eqs. (A10) and (A11)). Finally, $\int \rho \partial V_0/\partial V_1 da$ is expressed in terms of the charge, and its "center of mass", within the triangle (Eq. (A12), (A13)), and the contributions from all triangles immediately surrounding point 1 are added up to give the difference equation (A14).

To show that
$$\int \epsilon \vec{E}_4 \partial \vec{E}_0/\partial V_1 da = 0 , \tag{A5}$$

it is sufficient to prove that statement to be correct for the case where ρ is a δ-function. It is furthermore clear that since V_0 is a linear func-

tion of x,y, $\vec{E}_0$, and with it $\partial\vec{E}_0/\partial V_1$, is not dependent on x or y, so that we have to consider only $\int\vec{E}_4 da$. It is convenient to break this integral up into two parts: one integral over an infinitesimal disc surrounding the singularity, and the other over the rest of the triangle. Since $|\vec{E}_4| \sim 1/r$ for sufficiently small distance r from the singularity, the integral over the infinitesimal disc goes to zero like the linear dimension of the disc. The other integral is easily converted to a line integral:

$$\int\vec{E}_4 da = -\int\left(\vec{e}_x \frac{\partial V_4}{\partial x} + \vec{e}_y \frac{\partial V_4}{\partial y}\right) dx\, dy = \vec{e}_y \oint V_4\, dx - \vec{e}_x \oint V_4\, dy$$

$$\int\vec{E}_4 da = (\vec{e}_x \times \vec{e}_y) \times \oint V_4\, d\vec{s} \; .$$

This line integral has to be taken over the boundary of the region under consideration, i.e. the sides of the triangle and the circumference of the infinitesimal disc. The former integral is zero because $V_4 = 0$ on the sides of the triangle, and the latter integral vanishes with r since V_4 behaves like $\ln r$, and $\int|d\vec{s}|$ like r.

To evaluate the remaining two integrals in Eq. (A4), we have to find

$$\partial V_0/\partial V_1 = \underset{dV_1 \to 0}{\text{Lim}} \; [(V_0(x, y, V_1 + dV_1, V_2, V_3) - V_0(x, y, V_1, V_2, V_3))/dV_1]$$

Since $V_0(x, y, V_1, V_2, V_3)$ is a linear function of x and y, assuming the values V_1, V_2, V_3 at the corners of the triangle, $\partial V_0/\partial V_1$ becomes (see Fig. A2):

$$\partial V_0/\partial V_1 = V_0(x, y, dV_1, 0, 0)/dV_1 = d_1/h_1 \; . \tag{A6}$$

Multiplying numerator and denominator of that fraction by b_1 gives as

alternate form

$$\partial V_0/\partial V_1 = 2a_1/2a = \left(x(y_2 - y_3) + x_2(y_3 - y) + x_3(y - y_2)\right)/2a, \quad (A7)$$

where a is the area of the total triangle, and a_1 is the area of the partial triangle indicated in Fig. A2.

Introducing now the unit vectors $\vec{e}_1$, $\vec{e}_2$, $\vec{e}_3$ as indicated in Fig. A3, it follows from Eq. (A6) that

$$\partial \vec{E}_0/\partial V_1 = \vec{e}_1/h_1 , \quad (A8)$$

and consequently

$$\vec{E}_0 = \vec{e}_1 V_1/h_1 + \vec{e}_2 V_2/h_2 + \vec{e}_3 V_3/h_3 . \quad (A9)$$

Because $\vec{E}_0$ is independent of x,y, it follows that

$$\int 2\vec{E}_0 \partial \vec{E}_0/\partial V_1 \cdot da = h_1 b_1 \cdot \frac{1}{h_1}\left(\frac{V_1}{h_1} - \frac{V_2 \cos\alpha_3}{h_2} - \frac{V_3 \cos\alpha_2}{h_3}\right) ,$$

$$\int 2\vec{E}_0 \partial \vec{E}_0/\partial V_1 \cdot da = V_1 \cdot \frac{b_1}{h_1} - V_2 \cdot \frac{\cos\alpha_3}{h_2/b_1} - V_3 \frac{\cos\alpha_2}{h_3/b_1} .$$

From Fig. (A4) follows $h_2/b_1 = \sin\alpha_3$, and from Fig. (A5) follows $b_1/h_1 = \cot\alpha_2 + \cot\alpha_3$, giving

$$\int \varepsilon \vec{E}_0 \partial \vec{E}_0/\partial V_1 \cdot da = \frac{1}{2}\left(V_1(\cot\alpha_2 + \cot\alpha_3) - V_2 \cot\alpha_3 - V_3 \cot\alpha_2\right) \cdot \varepsilon . \quad (A10)$$

While this form is very well suited for interpreting the individual contributions in terms of the geometry of the triangle, for a computer program one obviously has to express the cotangents by the coordinates of the corners of the triangle. One can clearly write (see Fig. A4)

$$\cot\alpha_3 = \frac{b_1 b_2 \cos\alpha_3}{b_1 b_2 \sin\alpha_3} .$$

Since the numerator equals the scalar product of the vectors connecting point 3 to points 1 and 2, and the denominator equals twice the area of the triangle, we get

$$\cot \alpha_3 = \frac{(x_1 - x_3)(x_2 - x_3) + (y_1 - y_3)(y_2 - y_3)}{2a} . \qquad (A11)$$

To evaluate $\int \rho \partial V_0 / \partial V_1 da$, we use the explicit form for $\partial V_0 / \partial V_1$ given by Eq. (A7). It is also convenient to use the "center of mass" coordinates x,y of the charge distribution ρ in the triangle:

$$\int \bar{x} = \int x\rho da/q_0; \quad \bar{y} = \int y\rho da/q_0; \quad q_0 = \int \rho da . \qquad (A12)$$

To prevent the artificial "disaster" of the line charge q_0 being zero from occurring, one has to treat the effects from charges of different signs separately, which is done in the computer program.

Using Eq. (A12) in Eq. (A7) yields for the line charge q_1 associated with point 1 of the triangle under consideration:

$$q_1 = \int \rho \partial V_0 / \partial V_1 da = q_0 \frac{\bar{x}(y_2 - y_3) + x_2(y_3 - \bar{y}) + x_3(\bar{y} - y_2)}{2a} . \qquad (A13)$$

From the geometrical interpretation of q_1/q_0 as the ratio of areas of triangles (see Fig. A2) it is clear that $q_1 + q_2 + q_3 = q_0$, where q_2 and q_3 are the line charges associated with points 2 and 3 when optimization of T with respect to V_2, V_3 is considered. It is furthermore clear that the "center of mass" of the line charges q_1, q_2, q_3 deposited at the corners of the triangle coincides with the "center of mass" of the ρ-distribution. To show this explicitly, we need to consider only

$$\sum_3 x_1 q_1 / q_0 = \bar{x} \sum_3 x_1 (y_2 - y_3)/2a + \bar{y} (\sum_3 x_1 x_3 - \sum_3 x_1 x_2)/2a + (\sum_3 x_1 x_2 y_3 - \sum_3 x_1 x_3 y_2)/2a .$$

The factor multiplying $\bar{x}$ is clearly one, and the two differences of the

cyclical sums are obviously zero.

When optimizing T (Eq. A3) with respect to the potential at point 1, one obtains contributions according to Eqs. (A4, A5, A10, A11, A12, A13) from every triangle surrounding point 1. The potential of every point next to point 1 makes two contributions to $\partial T/\partial V_1$, one from each triangle that has the line connecting point 1 with its neighbor as a side. Instead of ordering the terms coming from Eq. (A10), (A13) according to triangles, it is more convenient to order them according to the points surrounding point 1. Using a notation explained in Fig. (A6), we get

$$\sum_6 (V_1 - V_n) \; (\varepsilon_{n+} \cot \alpha_{n+} + \varepsilon_{n-} \cot \alpha_{n-}) \cdot \tfrac{1}{2} = \sum_6 q_m \; .$$

One should notice that the dielectric constant ε associated with each triangle appears twice in this equation, once as ε_{n+}, and once as $\varepsilon_{(n+1)-} = \varepsilon_{n+}$. Defining the weights

$$W_n = (\varepsilon_{n+} \cot \alpha_{n+} + \varepsilon_{n-} \cot \alpha_{n-})/2 \; ,$$

we get:

$$V_1 \sum_6 W_n = \sum_6 V_n W_n + \sum_6 q_m \tag{A14}$$

The weights are, for the applications in this report, dependent only on geometry and need therefore to be computed only once. The total line charge $\sum_6 q_m$ associated with the point under discussion needs to be recalculated only, but always, when the charge distribution in the triangles changes.

APPENDIX B

Variational Principle for the Electrostatic Equations

We consider the quantity

$$T = \int [\epsilon(\vec{E})^2 - 2\rho V]dv , \tag{B1}$$

with $\vec{E}$ defined by

$$\vec{E} \equiv -\text{grad } V , \tag{B2}$$

and the volume integral extending over all space.

We now introduce

$$V = V_0 + \gamma V_1 \tag{B3}$$

with γ representing a space coordinate-independent scalar quantity used for "bookkeeping" purposes only. Using this in Eqs. (B1) and B2), and expanding in γ, we get

$$T = T_0 + \gamma T_1 + \gamma^2 T_2 \tag{B4}$$

with

$$T_0 = \int [\epsilon(\vec{E}_0)^2 - 2\rho V_0]dv$$

$$T_1 = -2\int (\epsilon\vec{E}_0 \text{grad } V_1 + \rho V_1)dv \tag{B5}$$

$$T_2 = \int \epsilon(\text{grad } V_1)^2 dv . \tag{B6}$$

Using the identity

$$\epsilon\vec{E} \text{ grad } V_1 = \text{div } (\epsilon\vec{E}_0 V_1) - V_1 \text{ div } \epsilon\vec{E}_0$$

in Eq. (B5), we get

$$T_1 = 2 \int (\text{div } \epsilon\vec{E} - \rho) V_1 dv - 2\int \text{div } (\epsilon\vec{E}_0 V_1) \cdot dv .$$

The second integral in this equation can be replaced by a surface integral over $\varepsilon \vec{E}_0 V_1$, which vanishes since $\vec{E}_0$ goes to zero faster than the surface goes to infinity (provided the net charge of the total system is zero). We therefore get:

$$T_1 = 2 \int (\text{div } \varepsilon \vec{E}_0 - \rho) V_1 \, dv .$$

(B7)

Since T_2 is obviously not negative, we come to the conclusion that if

$$\vec{E}_0 = -\text{grad } V_0; \quad \text{div } \varepsilon \vec{E}_0 = \rho$$

(B8)

T has a minimum, i.e. however one modifies V_0, T will always increase. Conversely, the potential that gives the minimum value for T must satisfy Eq. (B8). When dealing with two-dimensional fields, the volume integral can obviously be replaced by a surface integral over the two-dimensional geometry, and if we now drop the subscript 0, the variational principle takes the form used in Eqs. (A1, A2, A3).

APPENDIX C

Evaluation of $\int e^V da$ and $\int e^V z\,da$ for electron deposition

It has been shown in Appendix A (see Eq. (A12)) that for proper deposition of charges in a triangle, we have to know the total charge, and its "center of mass", for every triangle. For Boltzmann electrons, with a charge density proportional to exp (scalar potential/Ve) (see section 3a, 3c), this requires calculation of $\int e^V da$, $\int e^V z\,da$ if we introduce the argument of the exponential as new variable.

The derivation of the expressions for these integrals is simplified if we discuss the more general integral

$$I = \int F''(v)\, da. \tag{C1}$$

We assume that v is a linear function of x and y

$$v = \alpha x + \beta y + \delta , \tag{C2}$$

and the primes indicate differentiation with respect to v. Assuming temporarily that $\alpha \neq 0$, and that the values v_1, v_2, v_3 that v assumes at the three vertices of the triangle are all different from each other and not too small, the value for I can be obtained in the following way (see also Appendix D):

$$I = \frac{1}{\alpha} \int \frac{\partial F'}{\partial x} \cdot dx\,dy = \frac{1}{\alpha} \oint F'\,dy = \frac{1}{\alpha} \sum_{3}^{2} \int_{1} \frac{dy}{dv} \cdot F'\,dv .$$

Since $dy/dv = $ constant along every side of the triangle, we get, with $F(v_n) = F_n$:

$$I = \frac{1}{\alpha} \sum_{3} \frac{y_2 - y_1}{v_2 - v_1} (F_2 - F_1) = \frac{1}{\alpha} \sum_{3} F_2 \left(\frac{y_2 - y_1}{v_2 - v_1} - \frac{y_3 - y_2}{v_3 - v_2} \right) .$$

Bringing the two contributions of the bracket in the last sum onto the common denominator, the terms in the numerator proportional to β cancel each other, leaving only terms proportional to α. Their sum is easily identified as $-\alpha \cdot 2a$, where a equals the area of the triangle. We therefore get

$$I = 2a \sum_3 F_1/[(v_2 - v_1)(v_3 - v_1)] \ . \tag{C3}$$

In view of the formulas for the first moments for the case $F = e^v$, it is convenient for evaluation of (C3) to introduce the two sets of cyclical quantities

$$\mu_1 = 1/(v_2 - v_3) \tag{C4}$$

and

$$G_1 = F_1 \mu_2 \mu_3 \ , \tag{C5}$$

giving for Eq. (C3)

$$I = -2a \sum_3 G_1 \ . \tag{C6}$$

To get expressions for the moment of a function, we consider

$$J_x = \int F''' \ x \, da = \frac{\partial}{\partial \alpha} \int F'' \ da = \frac{\partial}{\partial \alpha} I \ ,$$

and obtain $J_x = \sum_3 x_1 \, \partial I/\partial v_1$, or more generally, with $z = x + iy$,

$$J_z = \sum_3 z_1 \frac{\partial}{\partial v_1} I \ . \tag{C7}$$

With Eqs. (C4, C5, C6) we obtain the explicit expression

$$J_z = -2a \sum_3 z_1 (F_1' \ \mu_2 \mu_3 + G_1 \ (\mu_2 - \mu_3) - G_2 \mu_3 + G_3 \mu_2) \ . \tag{C8}$$

For the specific case $F = e^v$, we get

$$J_z = -2a \sum_3 z_1 [G_1(1 + \mu_2 - \mu_3) - G_2 \mu_3 + G_3 \mu_2] \ , \tag{C9}$$

with

$$G_1 = e^{v_1} \mu_2 \mu_3 \ . \tag{C10}$$

It should be pointed out that if one wants the integral and moment of the same given function, the function F used in Eq. (C5) in conjunction with Eq. (C7) is the derivative of the function F used in Eq. (C5) in conjunction with Eq. (C6). The notation introduced in Eq. (C5) is therefore convenient only for the case of interest here, namely $F = e^v$. It is furthermore convenient to write

$$\exp(v) = \exp(\bar{v}) \cdot \exp(v - \bar{v}) \ , \tag{C11}$$

with

$$\bar{v} = \frac{1}{3}(v_1 + v_2 + v_3)_{original} \ , \tag{C12}$$

and pull the factor $\exp(\bar{v})$ outside all integrals. The function v then entering the integrands has the property

$$v_1 + v_2 + v_3 = 0 \ . \tag{C13}$$

This condition, which will be used throughout the rest of this Appendix, has to be used with some caution: for instance, Eq. (C13) can be applied <u>after</u> the operation on the right side of Eq. (C7) has been carried out, but not before.

Equations (C6, C9, C10) are not usable when two values of v entering these equations are identical, or when all values of v are zero. This means that when the difference between two values of v is sufficiently small, or when the absolute values of all v's are sufficiently small, round-off errors become so large that one has to use special expressions suited for these two cases. We will start with the case where two values of v, which we assume to be v_1 and v_2, satisfy

$$|v_2 - v_1| \ll 1 \ ,$$

but <u>without</u> at the same time satisfying $|v_1 + v_2| = |v_3| \ll 1$. To obtain the expressions for I and its derivatives, it is convenient to introduce the following abbreviations:

$$\gamma = (v_2 - v_1)/2 \tag{C14}$$

$$C = \cosh\gamma \; ; \; S = \sinh\gamma \tag{C15}$$

$$v_4 = \frac{3}{2}v_3 . \tag{C16}$$

With Eq. (C13), one then gets

$$v_2 = -v_3/2 + \gamma \; ; \; v_1 = -v_3/2 - \gamma \tag{C17}$$

$$v_3 - v_2 = v_4 - \gamma \quad ; \; v_3 - v_1 = v_4 + \gamma \tag{C18}$$

$$\exp v_2 = e^{-v_3/2} \cdot (C + S); \; \exp v_1 = e^{-v_3/2} (C - S) \tag{C18}$$

Using this notation in Eqs. (C4), (C6), (C9), and (C10), one obtains after some manipulation

$$I = \frac{2a\,e^{-v_3/2}}{v_4^2 - \gamma^2} \left(e^{v_4} - C - v_4 \frac{S}{\gamma} \right) \tag{C19}$$

$$\partial I/\partial v_3 = \frac{2a\,e^{-v_3/2}}{(v_4^2 - \gamma^2)^2} \left(2v_4 C + (v_4^2 + \gamma^2)\frac{S}{\gamma} + (v_4^2 - 2v_4 - \gamma^2)e^{v_4} \right) \tag{C20}$$

To obtain an easily usable expression for $\partial I/\partial v_1$ is not as straightforward as it is to get Eq. (C19), (C20). To show how our particular form of the result, Eq. (C21), is derived, we reproduce some intermediate steps:

$$\partial I/\partial v_1 = \frac{a \cdot e^{-v_3/2}}{v_4^2 - \gamma^2} \left(\frac{2e^{v_4}}{v_4 + \gamma} + \frac{K}{2\gamma^2} \right)$$

$$K = (C - S) \cdot 2\gamma \cdot (v_4 - \gamma) \left(\frac{1}{v_4 + \gamma} + 1 + \frac{1}{2\gamma} \right) - (C + S)(v_4 + \gamma)$$

$$K = (C - S)(v_4 - \gamma) \left(\frac{1}{v_4 + \gamma} + 1 \right) \cdot 2\gamma - 2\gamma C - 2\gamma v_4 \cdot S/\gamma$$

$$K/2\gamma = -C - v_4 S/\gamma + (C - S) \left(v_4 + \frac{v_4^2 + \gamma^2}{v_4^2 - \gamma^2} - \gamma \left(1 + \frac{2v_4}{v_4^2 - \gamma^2} \right) \right)$$

$$K/2\gamma = v_4 (C - S/\gamma) + C \cdot \frac{2\gamma^2}{v_4^2 - \gamma^2} - S \left(v_4 + \frac{v_4^2 + \gamma^2}{v_4^2 - \gamma^2} \right) - \gamma(C - S) \left(1 + \frac{2v_4}{v_4^2 - \gamma^2} \right)$$

$$\partial I/\partial v_1 = \frac{a e^{-v_3/2}}{v_4^2 - \gamma^2} \left(\frac{2e^{v_4}}{v_4 + \gamma} + v_4 \frac{C - S/\gamma}{\gamma} + C \frac{2v}{v_4^2 - \gamma^2} - \frac{S}{\gamma} \left(v_4 + \frac{v_4^2 + \gamma^2}{v_4^2 - \gamma^2} \right) - \right.$$

$$\left. (C - S) \left(1 + \frac{2v_4}{v_4^2 - \gamma^2} \right) \right) . \tag{C21}$$

Since $|\gamma| \ll 1$, it is clear that in Eqs. (C19 - C21), one should use the first terms of the power series for S/γ, $(C - S/\gamma)/\gamma$, to express these functions and S, C.

If one displaces the origin of the coordinate system, it follows immediately from the definition of J_z and Eq. (C7) that $\sum_3 \partial I/\partial v_1 = I$, and we use this relation to obtain $\partial I/\partial v_2$.

$$\partial I/\partial v_2 = I - \partial I/\partial v_1 - \partial I/\partial v_3 . \tag{C22}$$

We now turn to the case where the largest of the absolute values of v_1, v_2, v_3, is small compared to one. It is then convenient to expand the exponential in $\int e^v da$, $\int e^v z da$, into a power series, and then integrate the first few terms individually. We therefore have to evaluate

$$I_n = \int v^n da \tag{C23}$$

and

$$J_{n,z} = \int v^n z \, da \quad . \tag{C24}$$

for $n = 0, 1, 2, \text{---}$.

With Eqs. (C1) and (C3) we obtain

$$I_n = \frac{2a}{(n+1)(n+2)} \sum_3 v_1^{n+2} / (v_2 - v_1)(v_3 - v_1) \quad .$$

To make this expression suitable for evaluation, we rewrite this as

$$-(v_1 - v_2)(v_2 - v_3)(v_3 - v_1) \cdot (n+1)(n+2) I_n / 2a = v_1^{n+2}(v_2 - v_3) + v_2^{n+2}(v_3 - v_1) +$$

$$v_3^{n+2}(v_1 - v_2) \quad .$$

The right side of this equation is obviously zero for $v_1 - v_2 = 0$, $v_2 - v_3 = 0$, $v_3 - v_1 = 0$, i.e. it is possible to factor these terms out. We do this by using several times the explicit expression for the geometric sum, and start by rewriting the right side of the last equation as

$$v_3(v_2^{n+2} - v_1^{n+2}) + v_1 v_2(v_1^{n+1} - v_2^{n+1}) + v_3^{n+2}(v_1 - v_2)$$

Pulling out $v_2 - v_1$, and then continuing the same process, we get

$$(v_2 - v_3)(v_3 - v_1)(n+1)(n+2) I_n / 2a = v_3(v_2^{n+1} + \sum_0^n v_1^{n+1-\nu} v_2^{\nu}) - v_2 \sum_0^n v_1^{n+1-\nu} v_2^{\nu} - v_3^{n+2}$$

$$= (v_3 - v_2) \sum_0^n v_1^{n+1-\nu} v_2^{\nu} - v_3(v_3^{n+1} - v_2^{n+1})$$

$$(v_1 - v_3)(n+1)(n+2) I_n / 2a = \sum_0^n v_1^{n+1-\nu} v_2^{\nu} - \sum_0^n v_3^{n+1-\nu} v_2^{\nu} = \sum_0^n (v_1^{n+1-\nu} - v_3^{n+1-\nu}) v_2^{\nu}$$

$$I_n = \frac{2a}{(n+1)(n+2)} H_{3,n}(v_1, v_2, v_3) = \int v^n da \quad . \tag{C25}$$

$$H_{3,n}(v_1, v_2, v_3) = \sum_{\nu=0}^{n} \sum_{\mu=0}^{n-\nu} v_1^{n-\nu-\mu} v_3^{\mu} v_2^{\nu} \tag{C26}$$

$H_{3,n}$ is the homogeneous polynomial of the three variables v_1, v_2, v_3 of order $\underline{n}$ with all coefficients equal to one. Despite the fact that this polynomial has $(n+1)(n+2)/2$ terms, it is easily evaluated with a method patterned after Horner's method for the evaluation of a polynomial of a single variable: by splitting $H_{3,n}$ into an addend $H_{2,n}$ that depends only on v_1, v_2, and representing the remainder by v_3 times a factor that is obviously $H_{3,n-1}$, and then representing $H_{2,n}$ in the same manner, one arrives at the following algorithm:

$$\left. \begin{aligned} H_{1,n} &= v_1 H_{1,n-1}; \\[2mm] H_{2,n} &= H_{1,n} + v_2 H_{2,n-1} \\[2mm] H_{3,n} &= H_{2,n} + v_3 H_{3,n-1} \\[2mm] n &= 2, 3, \ldots \end{aligned} \right\} \tag{C27}$$

With the following initial conditions:

$$H_{1,1} = v_1; \quad H_{2,1} = H_{1,1} + v_2; \quad H_{3,1} = H_{2,1} + v_3. \tag{C28}$$

This recursion formula requires only $3(n-1)$ multiplications and $2n$ additions to calculate $H_{3,n}$.

A convenient alternate method of evaluating $H_{3,n}$ is obtained by applying Eq. (C13) to the explicit expressions of $H_{3,n}$. This leads to

$$H_{3,0} = 1$$

$$H_{3,1} = 0$$

$$H_{3,2} = (v_1^2 + v_2^2 + v_3^2)/2$$

$$H_{3,3} = v_1 v_2 v_3$$

$$H_{3,4} = v_1^2 v_2^2 + v_2^2 v_3^2 + v_3^2 v_1^2 \ . \tag{C29}$$

With the $H_{3,n}$ calculated, we finally get

$$\int e^V \, da = 2a \sum_n H_{3,n}/(n+2)! \tag{C30}$$

From Eqs. (C24, C7, C25) follows

$$\int v^n z \, da = \frac{2a}{(n+1)(n+2)(n+3)} \sum_3 z_1 \frac{\partial}{\partial v_1} H_{3,n+1} \tag{C31}$$

The derivative of H_3 with respect to v_3 can be obtained from the last of Eqs. (C27):

$$\partial H_{3,n}/\partial v_3 = H_{3,n-1} + v_3 \, \partial H_{3,n-1}/\partial v_3 \ . \tag{C32}$$

Since $H_{3,n}$ is completely symmetrical in v_1, v_2, v_3, the explicitly appearing variable v_3 in Eq. (C32) can be replaced by v_1 or v_2, thus giving a general recursive method to calculate the needed derivatives.

As done above, one can also obtain explicit expressions for the derivatives by carrying out the derivatives and then using Eq. (C13). Doing that gives

$$\partial H_{3,0}/\partial v_1 = 0$$

$$\partial H_{3,1}/\partial v_1 = 1$$

$$\partial H_{3,2}/\partial v_1 = v_1 \tag{C33}$$

$$\partial H_{3,3}/\partial v_1 = v_1^2 + v_2^2 + v_3^2 + v_2 v_3$$

$$\partial H_{3,4}/\partial v_1 = 2v_1 v_2 v_3 + v_1 (v_1^2 + v_2^2 + v_3^2) \ ,$$

and one obtains

$$\int e^V z \, da = 2a \sum_n \sum_3 z_1 \, \partial H_{3,n} / \partial v_1 \cdot \frac{1}{(n+3)!} \qquad (C34)$$

We can now summarize the procedure to calculate the desired integrals:

1) Carry through the normalization leading to Eq. (C13)

2) If the largest of the absolute values of v_1, v_2, v_3 is smaller than a predetermined number, go to 3, if not go to 4.

3) Calculate the $H_{3,n}$ and their derivatives with Eqs. (C27, C28, C32), or Eqs. (C29, C33), and use them in Eqs. (C30, C34).

4) If the smallest of the absolute values of $v_1 - v_2$, $v_2 - v_3$, $v_3 - v_1$ is smaller than a predetermined number, go to 5, if not go to 6.

5) Order v_1, v_2, v_3, without changing the cyclical order, so that $|v_1 - v_2|$ is the smallest of the absolute values of the differences of the v's. Calculate $I = \int e^V da$ and $J_z = \int e^V z \, da$ with Eqs. (C19, C20, C21, C22, C7).

6) Calculate I and J_z with Eqs. (C4, C10, C6, C9).

APPENDIX D

Integration of functions over triangle area; the area of a triangle; and cyclical ordering

When integrating functions over triangle areas, the following formulas will be used (see Fig. D1):

$$\int \frac{\partial F}{\partial x} \, dxdy = \int [F(x_R, y) - F(x_L, y)] \, dy$$

$$\int \frac{\partial F}{\partial x} \, dxdy = \oint F \, dy \; . \tag{D1}$$

$$\int \frac{\partial F}{\partial y} \, dxdy = \int [F(x, y_T) - F(x, y_B)] \, dx$$

$$\int \frac{\partial F}{\partial y} \, dxdy = - \oint F \, dx \; . \tag{D2}$$

To calculate the area, we use Eq. (D1) with $\partial F/\partial x = 1$. Assuming the vertices 1,2,3 (see for instance, Fig. A1) to be in correct cyclical order, i.e., going from 1 to 2 to 3 to 1 representing going around the triangle in counter-clockwise direction, we get for the area a of the triangle:

$$a = \oint x \, dy = \sum_3 \int_1^2 \frac{dy}{dx} \cdot x \, dx = \sum_3 \frac{y_2 - y_1}{x_2 - x_1} \cdot \frac{x_2^2 - x_1^2}{2}$$

$$2a = \sum_3 (y_2 - y_1)(x_1 + x_2) = \sum_3 x_1(y_2 - y_1) + \sum_3 x_1(y_1 - y_3)$$

$$2a = \sum_3 x_1(y_2 - y_3) = -\sum_3 y_1(x_2 - x_3) \tag{D3}$$

Equation (D3) can be used to check whether a sequence of three points is cyclically correct: $a > 0$ is necessary and sufficient for order of points

to be cyclically correct; and $a < 0$ is necessary and sufficient for order of points to be cyclically incorrect. Should that be the case, one gets correct order by reversing the order of a pair of points.

APPENDIX E

Modification of curvature by conformal transformation

We first derive a formula for the curvature of a curve that is given by a parametric representation: Let t be a real parameter, and let the curve be given by $x(t)$ and $y(t)$, or, equivalently, $z(t)$. To obtain the curvature at $t = 0$, we expand z into a power series

$$z(t) = z_0 + \dot{z} \cdot t + \ddot{z}t^2/2 + \ldots$$

where $\dot{z}$, $\ddot{z}$, indicates the derivatives for $t = 0$. With

$$\dot{z} = |\dot{z}|e^{i\alpha_z} \tag{E1}$$

assumed to be non-zero, and

$$\ddot{z}e^{-i\alpha_z} = a + ib , \tag{E2}$$

we get

$$z(t) = z_0 + e^{i\alpha_z} (|\dot{z}|t + (a + ib)t^2/2 + \ldots)$$

$e^{i\alpha_z}$ indicates the direction of the tangent to the curve $z(t)$ at $t = 0$ for increasing values of t. We now introduce a local Cartesian coordinate system, ζ, η with its center at z_0 and the ζ axis parallel to $e^{i\alpha_z}$. In the vicinity of $t = 0$ the curve is then given by

$$\zeta = |\dot{z}| \cdot t + at^2/2 + \ldots ,$$

$$\eta = bt^2/2 + \ldots$$

For $t = 0$,

$$d\eta/d\zeta = \dot{\eta}/\dot{\zeta} = (bt + \ldots)/(|\dot{z}| + at + \ldots)$$

is zero, and the curvature k_z at $t = 0$ is therefore given by

$$k_z = d^2\eta/d\zeta^2 = \left(\frac{1}{\dot{\zeta}} \cdot \frac{d(\dot{\eta}/\dot{\zeta})}{dt}\right)_{t=0} = b/|\dot{z}|^2 .$$

With Eqs. (E1, E2) we get

$$k_z = \text{Im}(\ddot{z}\, e^{-i\alpha_z}/|\dot{z}|^2)$$

$$k_z = \text{Im}\left(\frac{\ddot{z}}{\dot{z}}\right)/|\dot{z}| . \tag{E3}$$

From the derivation it follows that $k_z > 0$ if the center of curvature is to the left of the tangent direction $e^{i\alpha_z}$.

If we map the z-plane conformally onto the w-plane with $w(z)$, w is also a function of t and Eq. (E3) is applicable:

$$k_w = \text{Im}\left(\frac{\ddot{w}}{\dot{w}}\right)/|\dot{w}| . \tag{E4}$$

If we indicate derivatives of w with respect to z by primes, we get

$$\dot{w} = w' \cdot \dot{z}$$

$$\ddot{w} = w'' \, \dot{z}^2 + w'\ddot{z} .$$

Assuming that w' and $z' = 1/w'$ are non-zero, we get

$$\ddot{w}/(\dot{w}|\dot{w}|) = \left(\frac{w''}{w'} \cdot \frac{\dot{z}}{|\dot{z}|} + \frac{\ddot{z}}{\dot{z}|\dot{z}|}\right)/|w'| .$$

With Eqs. (E4, E3, E1) we get one form of k_w:

$$k_w = \left[k_z + \text{Im}\left(\frac{w''}{w'} e^{i\alpha_z}\right)\right]/|w'| \tag{E5}$$

To obtain another expression for k_w, we solve Eq. (E5) for k_z, and then exchange all z and w, giving

$$k_w = |z'|k_z - \operatorname{Im}\frac{z''}{z'}\, e^{i\alpha_w} \quad . \tag{E6}$$

As before, curvatures are > 0 when the center of curvature is to the left of the tangent defined by direction of progression along the curve.

In addition to having the option of expressing k_z in terms of derivatives of z with respect to w, or w with respect to z, it can also be convenient to express the direction of the tangent in terms of either α_z or α_w. The relation between these two directions is obviously given by

$$e^{i\alpha_w}/e^{i\alpha_z} = w'/|w'| = |z'|/z' \quad , \tag{E7}$$

so that Eqs. (E5, E6, E7) allow to write the result in four different ways.

One can use the same technique to obtain the next higher order term, k_w', the change of the curvature per unit length along the tangent. Since we do not use these formulas in our discussions, but the reader may want to expand on the treatment in Appendix F, we give here the result without derivation:

$$k_w' = \left(k_z' + \operatorname{Im}\left[\left(\frac{w'''}{w'} - \frac{3}{2}\left(\frac{w''}{w'}\right)^2\right)e^{2i\alpha_z}\right]\right)/|w'|^2 \tag{E8}$$

$$k_w' = |z'|^2 k_z' - \operatorname{Im}\left[\left(\frac{z'''}{z'} - \frac{3}{2}\left(\frac{z''}{z'}\right)^2\right)e^{2i\alpha_w}\right] \quad . \tag{E9}$$

APPENDIX F

The one-dimensional diode, and its use as a test problem

We consider groups of ions with charge to mass ratios

$$e_n/m_n = a_n/2 \tag{F1}$$

emanating in the x-direction with current densities j_n from a flat emitter at $x = 0$. We assume that the scalar electric potential depends only on x. To avoid having to work with a function that is, at least in all the cases discussed here, always negative, we use the negative of the scalar potential, normalized to be zero at $x = 0$, to describe the electric field:

$$V(x) = -(\text{potential at } x - \text{potential at emitter}).$$

If N_n represents the particle density of group n, and v_n their velocity, conservation of the number of particles in group n requires

$$N_n \cdot v_n = \text{independent of } x,$$

or

$$n_n e_n v_n = j_n = \text{const.} \tag{F2}$$

If we also allow an electron charge density ρ_e, $\varepsilon_0 \, \text{div} \, \vec{E} = \text{charge density}$ gives

$$\varepsilon_0 V'' = \sum \frac{j_n}{v_n} - \rho_e \ . \tag{F3}$$

If we represent the initial energy of ions of group n by $e_n V_n$, energy conservation gives:

$$v_n = \sqrt{a_n} \cdot \sqrt{V + V_n} \ .$$

Assuming ρ_e to be a known function of V, Eq. (F3) becomes

$$V'' = \frac{1}{2}\frac{d(V'^2)}{dV} = \sum \frac{j_n/\varepsilon_0\sqrt{a_n}}{\sqrt{V + V_n}} - \frac{\rho_e(V)}{\varepsilon_0} \qquad (F4)$$

Integrating this over V gives, with

$$C(V) = \frac{2}{\varepsilon_0}\int_0^V \rho_e(V)\,dV \;, \qquad (F5)$$

$$b_n = 4j_n/\varepsilon_0\sqrt{a_n} \;: \qquad (F6)$$

$$V' = \left(V_0'^2 - C(V) + \sum b_n(\sqrt{V + V_n} - \sqrt{V_n})\right)^{\frac{1}{2}} \;. \qquad (F7)$$

V_0' represents the electric field at the emitter, and we assume for simplicity that $V_0' \geq 0$. From Eq. (F7) then follows:

$$x = \int_0^V \frac{dV}{\sqrt{V_0'^2 - C(V) + \sum b_n(\sqrt{V + V_n} - \sqrt{V_n})}} \qquad (F8)$$

For some discussions, it will be necessary to expand V'^2 into a power series in V for the case where all $V_n > 0$. If we write

$$C''(0) = \rho_e'(0) = \rho_{e,0}/V_e \;,$$

which is consistent with a Boltzmann distribution for the electrons ($\rho_e = \rho_{e,0}e^{-V/V_e}$, see Sect. 3a), we get from Eq. (F7);

$$V'^2 \approx V_0'^2 + g_1 V + g_2 V^2/2 \qquad (F9)$$

with

$$g_1 = \sum \frac{b_n}{2\sqrt{V_n}} - \frac{2}{\varepsilon_0}\rho_{e,0} = \frac{2}{\varepsilon_0}\sum(\rho_{n,0} - \rho_{e,0}) \qquad (F10)$$

$$g_2 = \frac{2}{\varepsilon_0} \frac{\rho_{e,0}}{V_e} - \sum \frac{b_n}{2\sqrt{V_n}} \frac{1}{2V_n} = \frac{1}{\varepsilon_0} \left(\frac{2\rho_{e,0}}{V_e} - \sum \frac{\rho_{n0}}{V_n} \right) . \qquad (F11)$$

In these expansions, ρ_{n0} represents the charge density from ion group n at the emitter, and Eq. (F9) is a good approximation when $(V/V_n)^2/8 \ll 1$, $(V/V_c)^2/6 \ll 1$.

To get an analytical test case, we follow Pierce's argument that leads to the "Pierce electrodes" as described in his book (ref. F1): If we remove all particles for $y > 0$, the flow characterized by Eq. (F8) is not perturbed provided we can construct an electrode structure in the $y > 0$ half-space that has the property that if for $y = 0$, the relationship between x and V is given by Eq. (F8), $E_y = 0$ for $y = 0$. To describe the vacuum fields for $y > 0$, it is advisable to augment the negative of the scalar potential, V, (which satisfies Laplace's equation for $y > 0$) by its harmonic conjugate, A, and form the analytic function of z

$$G(z) = V + iA \qquad (F12)$$

A is the (only necessary) component of the vector potential in the direction perpendicular to the x-y plane, and is related to E_x, E_y, by

$$E_x = \partial A/\partial y \; ; \quad E_y = -\partial A/\partial x .$$

It is also easily verified that

$$E^* = E_x - iE_y = G'(z) \qquad F13)$$

Since $G(z) = V + iA$ represents a conformal mapping of the V,A plane onto the z plane, and V = constant lines are perpendicular to the field lines, A = constant represent field lines.

From all this follows directly that the fields and potentials for $y > 0$ are given by Eqs. (F7) and (F8) if one replaces x by z and V by G.

Rewriting previously used equations this way, we obtain

$$2G'' = d(G'^2)/dG \qquad (F14)$$

$$G' = E^* = \sqrt{V_0'^2 - C(G) + \Sigma\, b_n(\sqrt{G+V_n} - \sqrt{V_n})} \qquad (F15)$$

$$z = \int_0^G \frac{dG}{G'} \quad . \qquad (F16)$$

Since, in the region of interest, G' is single-valued and does not have any singularities, it is indeed possible to find an electrode system that has the desired properties, and Fig. F2 depicts such a system: When the constants entering Eq. (F16) are specified, the shape of the continuation of the emitter electrode follows from Eq. (F16) by using as integration limits $G = 0 + iA$, with A increasing, starting from zero, up to A_{C1}, that point representing one corner of the geometry one wants to treat. Letting then V in $G = V + iA_{C1}$ monotonically increase up to V_{C2}, gives the shape of a field line, leading to another corner. Letting then A in $G = V_{C2} + iA$ decrease monotonically from A_{C1} to $A = 0$ gives the other electrode, which should then be continued parallel to the emitter for $y < 0$. If one introduces a limiting symmetry line some place below the x axis parallel to the x axis, one has specified a non-trivial test problem that can be run with FLOW and that has an analytical solution.

It is instructive to make some general statements about the electrodes, as well as to discuss a few special cases. Since we want to discuss curvatures of electrodes, it is worthwhile to introduce the notation used here into Eqs. (E6, E7): using the expression for $e^{i\alpha_w}$ given by Eq. (E7) in Eq. (E6), and replacing in Eq. (E6) z by G, and w by z, we obtain

$$k_z = |G'| \cdot [K_G - \text{Im} \left(\frac{G''}{G'^2} e^{i\alpha_G} \right)] \ . \tag{F17}$$

For the case of an electrode, $(V = \text{const.})$, we set $k_G = 0$ and $e^{i\alpha_G} = i$, and get

$$k_z = -|G'| \ \text{Re} \ (G'' /G'^2) \ . \tag{F18}$$

The following statements result directly from (F14, F15, F18) with little additional work, with the exception of the singularities for the curvatures mentioned below in Section 3a(2) and 3b(1)II. Calculations relating to these curvatures are carried out in Appendix G.

1. There is no solution for the one-dimensional diode (except the trivial solution $V = 0$ everywhere) when the electric field is zero at the emitter and the total charge density vanishes there also. We therefore exclude that case from the following considerations.

2. The angle between the tangent to every equipotential (electrode) and the x axis is $3/4 \cdot 90^\circ = 67.5^\circ$ for sufficiently large values of A.

3. Characteristics of equipotentials (electrodes) for vanishingly small values of Λ.

    a. $G' > 0$: (At emitter or anyplace downstream) initial angle α_{init} between tangent to electrode and x-axis $= 90^\circ$.

    (1) If all ion groups have non-zero energy, the initial curvature is given by $k_z = -(\rho_{tot}/\varepsilon_0)/G'$.

    (2) If one or more $V_n = 0$, $k_z < 0$ has a singularity for $V = 0$, because when a V_n goes to zero, the associated charge density goes to infinity. (This applies only to $V = 0$-electrode.)

b. $G' = 0$ ($V = 0$-electrode for case $V_0' = 0$)

    (1) At least one $V_n = 0$: $\alpha_{init} = 67.5^O$.

          I. If no electrons are present, and if all

              $V_n = 0$, the electrode is a straight line

              (Pierce electrode, see 4a).

          II. If electrons are present and/or at least

              one $V_n > 0$, $k_z < 0$ has a singularity.

    (2) All $V_n > 0$: $\alpha_{init} = 45^O$; $k_z = 0$ for $A \nmid 0$.

4. Closed expressions for $z(g)$ can be given when there are no

electrons and when there is only one ion species. (More than

one ion species, but all $V_n = 0$, is counted as one species only.)

a. $V_1 = 0$; $V_0 = 0$; $z = 4/3 \cdot 1/\sqrt{b} \cdot G^{3/4}$

    This is the original Pierce electrode system: The equi-

    potential $V = 0$ is obviously a straight line with $\alpha = 67.5^O$.

    The electrodes with $V > 0$ start with $\alpha_{init} = 90^O$ and have an

    initial curvature $k_z = - \sqrt{b} \, V^{-3/4}/4$.

b. $V_1 > 0$ leads to the following expression.

$$z = \frac{4V_1^{3/4}}{3\sqrt{b_1}} \left\{ \sqrt{\sqrt{1 + G/V_1} - a} \left(\sqrt{1 + G/V_1} + 2a \right) - \sqrt{1 - a} \, (1 + 2a) \right\}$$

$$\text{(F19)}$$

$$a = 1 - V_0'^{2}/b_1 \sqrt{V_1} \quad .$$

Because of its simplicity, this case was used with $a = 1$ as a test problem

before electrons were introduced, and the result is shown in Figs. (F1)

and (F2): Fig. F1 shows the vacuum equipotentials and the ion trajectories

in that field. Figure F2 shows equipotentials and ion trajectories after

the computation has converged.

When one discusses one dimensional diodes as we do here, one should never forget that the model "ions are always emitted in a direction perpendicular to the emitter surface" represents an assumption that is not realizable in the real world. While it may be possible to produce conditions where $G' = 0$ at the emitter, the cases that lead to singularities for the curvature of the continuation of the emitter electrode are to a stronger degree not realizable idealizations, and all configurations that are close to them have to be treated with a lot of caution.

APPENDIX G

Curvature of some equipotentials

We want to calculate the curvature of some equipotentials for very small values of Λ in the case where at least one ion species has $V_n = 0$. Lumping all ions with $V_n = 0$ into one group, for small enough $G = iA$, it is sufficient to represent G'^2 by

$$G'^2 = V_0'^2 + g_0\sqrt{G} + g_1 G \qquad (G1)$$

with g_1 resulting from electrons and ions with $V_n > 0$ given by Eq. (F10), and g_0 given by

$$g_0 = \sum_{\substack{\text{ions} \\ \text{with} \\ V_n = 0}} 4j_n/\varepsilon_0\sqrt{a_n} \quad .$$

With Eqs. (F18), (G1) and (F14), we get

$$k_z = -\frac{|G'|}{4} \operatorname{Re} \frac{1}{\sqrt{G}} \frac{g_0 + 2g_1\sqrt{G}}{V_0'^2 + g_0\sqrt{G} + g_1 G} \quad . \qquad (G2)$$

1. $V_0' > 0$; for small A, we get

$$k_z = -\frac{g_0}{4V_0'} \operatorname{Re} \frac{1}{\sqrt{iA}} = -\frac{1}{4\sqrt{2}} \cdot \frac{g_0}{V_0'\sqrt{A}} \quad . \qquad (G3)$$

giving a (weak) singularity for $A \to 0$. Together with Eq. (G1), we conclude that the initial tangent in the y-direction bends in the "singular" way expressed by Eq. (G3) in a new direction, approaching a n angle $\alpha = 67.5^{\circ}$ between tangent and x-axis.

2. $V_0' = 0$: for small A, we get

$$k_z = - \frac{\sqrt{g_0} \; \Lambda^{\frac{1}{4}}}{4} \; \mathrm{Re} \; \frac{1}{G} \; \frac{1 + 2 \; g_1 \sqrt{G}/b_0}{1 + g_1 \sqrt{G}/b_0}$$

$$k_z = - \frac{\sqrt{g_0} \; \Lambda^{\frac{1}{4}}}{4} \; \frac{g_1}{g_0} \; \mathrm{Re} \; \frac{1}{\sqrt{iA}} = - \frac{1}{4\sqrt{2}} \; \frac{g_1}{\sqrt{g_0} A^{\frac{1}{4}}} \tag{G4}$$

We again get a (weak) singularity for $A \to 0$. Together with Eq. (G1), we learn that from the initial value $\alpha = 67.5^\circ$, the tangent bends in the "singular" way expressed by Eq. (G3) to a new direction, tending toward $\alpha = 45$, only to ultimately return to 67.5° according to summary statement #2 in Appendix F.

APPENDIX H

Calculation of the electric field at the emitter

The calculation of the electric field at the emitters is contaminated by two errors: erroneous potentials at mesh points due to discretization, and errors introduced in calculating the electric field from the potential and the mesh geometry. We attack here the latter problem and will derive a formula that is better than just dividing a potential difference by a distance.

We discuss a triangle whose one side is part of the emitter surface, and want to find the relationship between the electric field V_o' at the emitter surface, on one hand, and the distance D of the third triangle point from the emitter, the potential difference V between that point and the emitter, and the other quantities characterizing the flow there. To do so, we use the model of the one dimensional diode discussed in Appendix F. Since there are at present no plans to introduce ions with initial velocity zero at emitters that require electric field calculation, we use Eq. (F9) to describe the electric field in the triangle. In Eq. (F6), defining the quantities b_n entering Eqs. (F10) and (F11), one has to use for j_n the current density component perpendicular to the emitter element, and for V_n the energy associated with the velocity component perpendicular to the emitter.

Introducing,

$$\left. \begin{array}{l} u = \sqrt{g_2/2} \ D \\[2mm] v = \sqrt{g_2/2} \ V \\[2mm] \beta = g_1 \ \sqrt{2g_2} \quad , \end{array} \right\} \qquad \text{(H1)}$$

integration of Eq. (F9) gives

$$u = \ln \frac{v + \beta + \sqrt{(v + \beta)^2 + V_0'^2 - \beta^2}}{\beta + V_0'} \quad .$$

Solving this for V_0' gives

$$V_0' = \frac{V - \frac{g_1}{g_2} (\cosh u - 1)}{D} \cdot \frac{u}{\sinh u} \tag{H2}$$

A different form, good for small u, is

$$V_0' = \frac{V - \frac{g_1 D^2}{4} \left(\frac{\sinh u/2}{u/2}\right)^2}{D} \cdot \frac{u}{\sinh u} \quad . \tag{H3}$$

These expressions are good approximations when Eq. (F9) is a good representation of Eq. (F7), i.e., when $(V/V_n)^2/8 \ll 1$; $(V/V_e)^2/6 \ll 1$.

APPENDIX J

Ion Trajectories

Since the scalar potential is computed at the mesh points of an irregular triangular mesh, computation of the ion trajectories is basically accomplished if one traces an ion from the intersection with one side of a triangle through the triangle to the next intersection with a side of the same triangle. Every traced ion is actually representative of a current (per unit length in the direction perpendicular to the x-y plane), and one needs therefore, in addition to "updating" information of initial conditions for the equations of motion, the total charge present in the triangle, and its "center of mass". To obtain the ion trajectory, we assume again that the electric field is constant within the triangle. After solving the trajectories first with only this electric field present, we then generalize that solution and take into account to first order a constant magnetic field in the direction perpendicular to the x-y plane. We use complex arithmetic to formulate and solve the trajectory equations.

If 2g represents the complex representation of the electric field multiplied by the charge to mass ratio of the ion, the equation of motion is:

$$\ddot{z} = 2g \tag{J1}$$

Indicating initial conditions by the subscript 0, we get from Eq. (J1):

$$\dot{z} = \dot{z}_0 + 2gt \ , \tag{J2}$$

$$z = z_0 + \dot{z}_0 t + gt^2 \ . \tag{J3}$$

The electric field is easily obtained from Eq. (A9):

$$\vec{E} = \sum_3 \vec{e}_2 \, V_2/h_2 = \sum_3 \vec{e}_2 \, b_2 \, V_2/(b_2 h_2)$$

Switching to complex representation, it is clear from Fig. (A3) and (A4) that

$$E = \sum_3 i(z_3 - z_1) V_2/(b_2 h_2) \ .$$

With $a = b_2 h_2/2$ representing the area of the triangle (Eq. (D3)), we get

$$E = \frac{i}{2a} \sum_3 V_1 \, (z_2 - z_3) = 2g \ (m/e) \ . \tag{J4}$$

To find the intersection of the trajectory, Eq. (J3), with one side of the triangle, say the one connecting point 1 to point 3, we set

$$z = z_0 + \dot{z}_0 t + g t^2 = z_1 + (z_3 - z_1) \cdot \mu \ .$$

The time of intersection follows from the condition that μ is real:

$$\mu |z_3 - z_1|^2 = (z_3 - z_1)^* \, (z_0 - z_1 + \dot{z}_0 t + g t^2) \ .$$

With

$$b_0 = \mathrm{Im}((z_0 - z_1)(z_3 - z_1)^*) \ ,$$

$$b_1 = \mathrm{Im}(\dot{z}_0 (z_3 - z_1)^*) \ ,$$

$$b_2 = \mathrm{Im} \, g(z_3 - z_1)^* \ ,$$

we obtain for the time t_4 of intersection of the trajectory, originating at z_0 on side 1-2, with side 1-3:

$$b_2 t_4^2 + b_1 t_4 + b_0 = 0$$

$$t_4 = -\frac{b_1}{2b_2} \pm \sqrt{\left(\frac{b_1}{2b_2}\right)^2 - \frac{b_0}{b_2}} \ .$$

When the expression under the square root is negative, an intersection does not exist. Among the existing intersections with all three sides of the triangle, one is obviously only interested in the one with the smallest positive time t_4. To avoid tests for the signs of t_4, it is easier to find the largest value of $1/t_4$, needing only to pick the largest of the three values

$$1/t_4 = - \frac{b_1}{2b_0} + \sqrt{\left(\frac{b_1}{2b_0}\right)^2 - \frac{b_2}{b_0}} \; . \tag{J5}$$

In the expression for the intersection with the side of the triangle from which the trajectory starts, $b_0 \equiv 0$ and Eq. (J5) has to be replaced by

$$1/t_4 = -b_2/b_1 \; . \tag{J6}$$

Having thus found the correct t_4 for the intersection, the new starting point and velocity are obtained by using t_4 for t in Eqs. (J2) and (J3).

In the following discussion of charge deposition, when talking about current charge, etc., it should be understood that these terms mean the mentioned quantity per unit length of the problem in the direction perpendicular to the x-y plane.

With each trajectory is associated a current I. The relation between I and the charge ρ per unit length of trajectory is obviously

$$I = \rho \cdot |\dot{z}| = \rho v = \rho ds/dt \; .$$

The total charge residing in a triangle is then given by

$$q_0 = \int \rho ds = I \cdot \int dt = I \cdot t_4 \; , \tag{J7}$$

and its "center of mass", $\bar{z}$, also needed for the solution of Poisson's

equation, is given by

$$\bar{z} \cdot q_0 = \int z \rho dt = I \int_0^{t_4} z dt \ ,$$

$$\bar{z} = \int_0^{t_4} z dt / t_4 \tag{J8}$$

With Eq. (J3), we obtain

$$\bar{z} = z_0 + \dot{z}_0 \, t_4 / 2 + g t_4^2 / 3 \ . \tag{J9}$$

When a homogeneous magnetic field B in the direction perpendicular to the x-y plane is present, the equation of motion becomes

$$\ddot{z} = 2g - iC\dot{z} \ . \tag{J10}$$

C is the cylcotron frequency (B times the charge to mass ratio) of the ion species under consideration. First integration of Eq. (J10) gives

$$\dot{z} = \dot{z}_0 + 2gt - iC(z - z_0) \ . \tag{J11}$$

While this equation can be integrated in closed form, this is not advisable since the solution involves trigonometric functions, and approximations have to be made anyway for the calculation of t_4. We therefore carry from now on only terms up to first order in C. It turns out that that is a good approximation as long as

$$(Ct_4)^2 / 6 \ll 1 \tag{J12}$$

With this approximation, we get from Eq. (J11):

$$z = z_0 + \dot{z}_0 t + g t^2 - iC(\dot{z}_0 t^2 / 2 + g t^3 / 3) \ . \tag{J13}$$

Defining, in addition to b_0, b_1, b_2 the quantities

$$b_3 = \text{Re} \ g(z_3 - z_1)^* / 3 \ ,$$

$$b_4 = \text{Re } z_0(\dot{z}_3 - z_1)^*/2 \; ,$$

the condition for intersection of line 1-3 becomes

$$b_2 t^2 + b_1 t + b_0 - C(t^3 b_3 + t^2 b_4) = 0 \; .$$

Introducing $1/t_4 = \omega_4$, we get

$$b_0 \omega_4^2 + b_1 \omega_4 + b_2 - C(b_4 + b_3/\omega_4) = 0$$

With ω_{40} representing the right side of Eq. (J5) or (J6), we get to first order in C

$$1/t_4 = \omega_{40} + C/\omega_{40} \cdot (b_3 + b_4 \omega_{40})/(b_1 + 2b_0 \omega_{40}) \; . \tag{J14}$$

With this value of t_4, the endpoint of the trajectory in the triangle is given by Eq. (J13), and the endpoint velocity follows from Eq. (J11) and (J13). The total charge deposition is again given by Eq. (J7), and its "center of mass" is obtained from Eqs. (J8) and (J13):

$$\bar{z} = z_0 + \dot{z}_0 t_4/2 + g t_4^2/3 - iC(2\dot{z}_0 t_4^2 + g t_4^3)/12 \; . \tag{J15}$$

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A1. A. Winslow, Ref. 3, and also UCRL-7784.

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    1954.
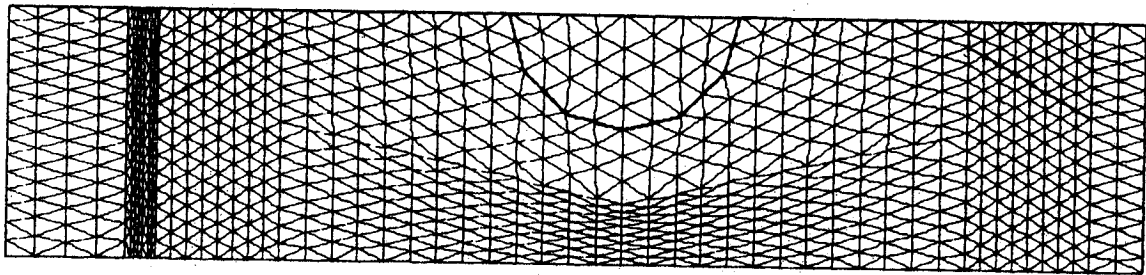
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Figure A1. Mesh plot.
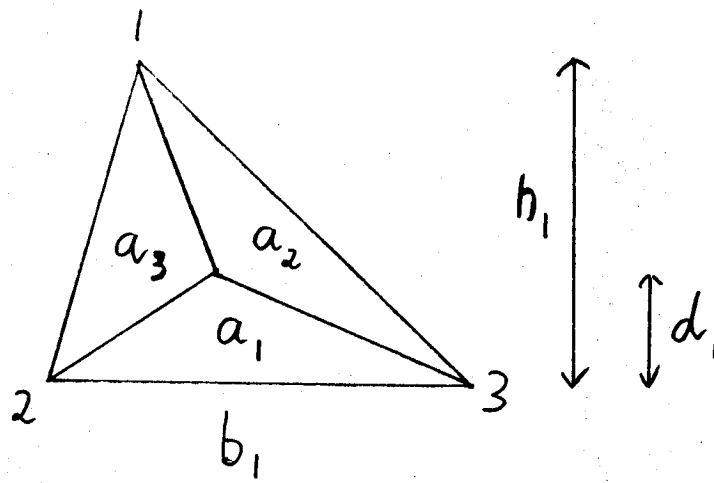
Figure A2.   Identification of quantities in a triangle.
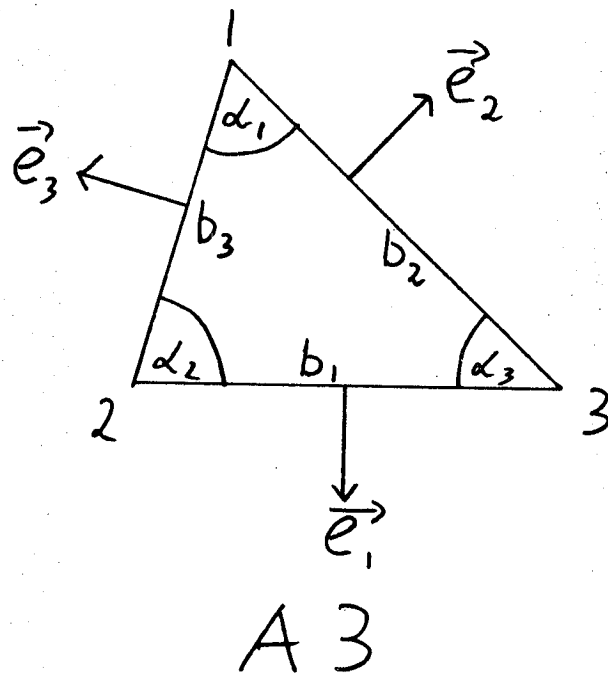
Figure A3. Identification of quantities in a triangle.
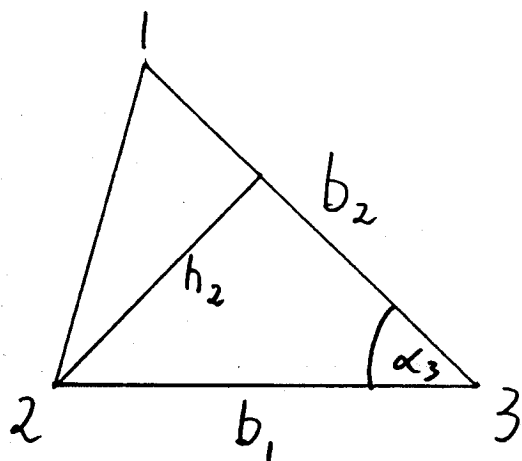
Figure A4. Identification of quantities in a triangle.
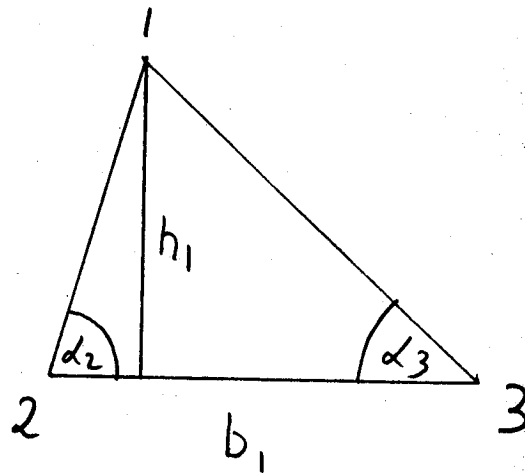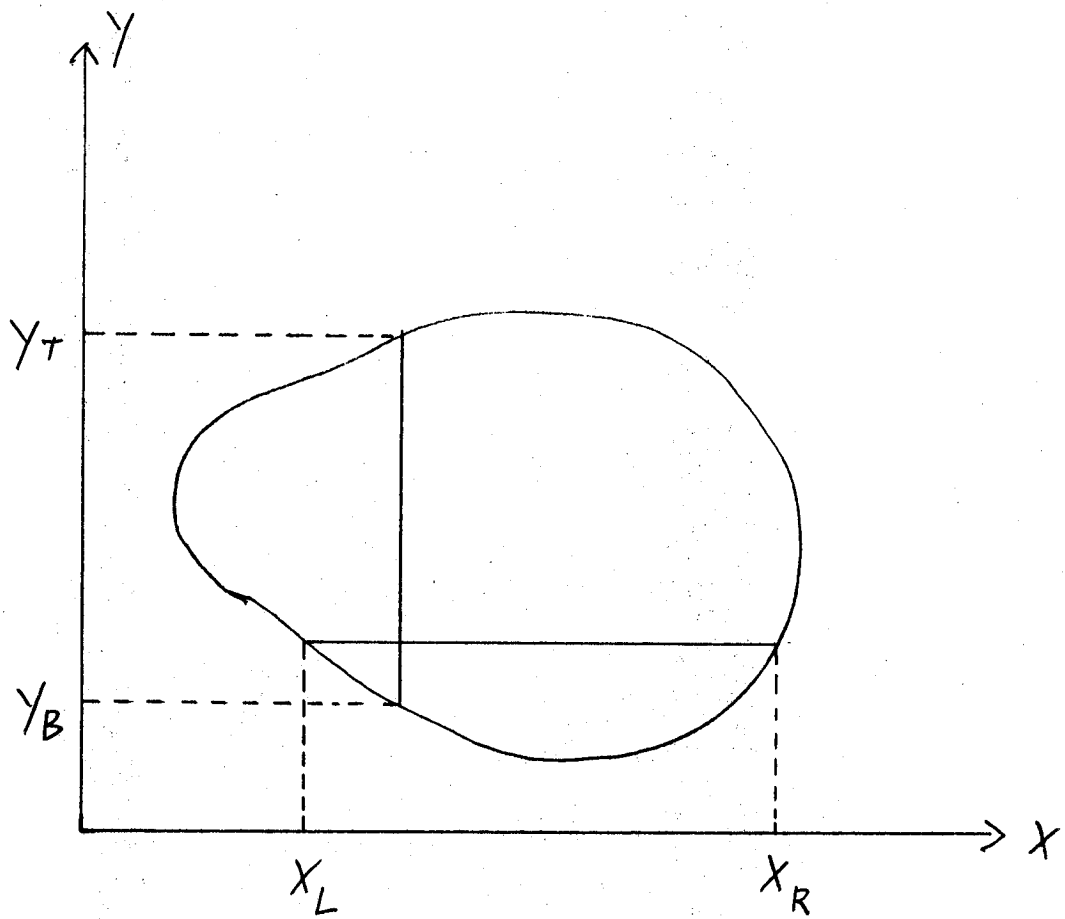
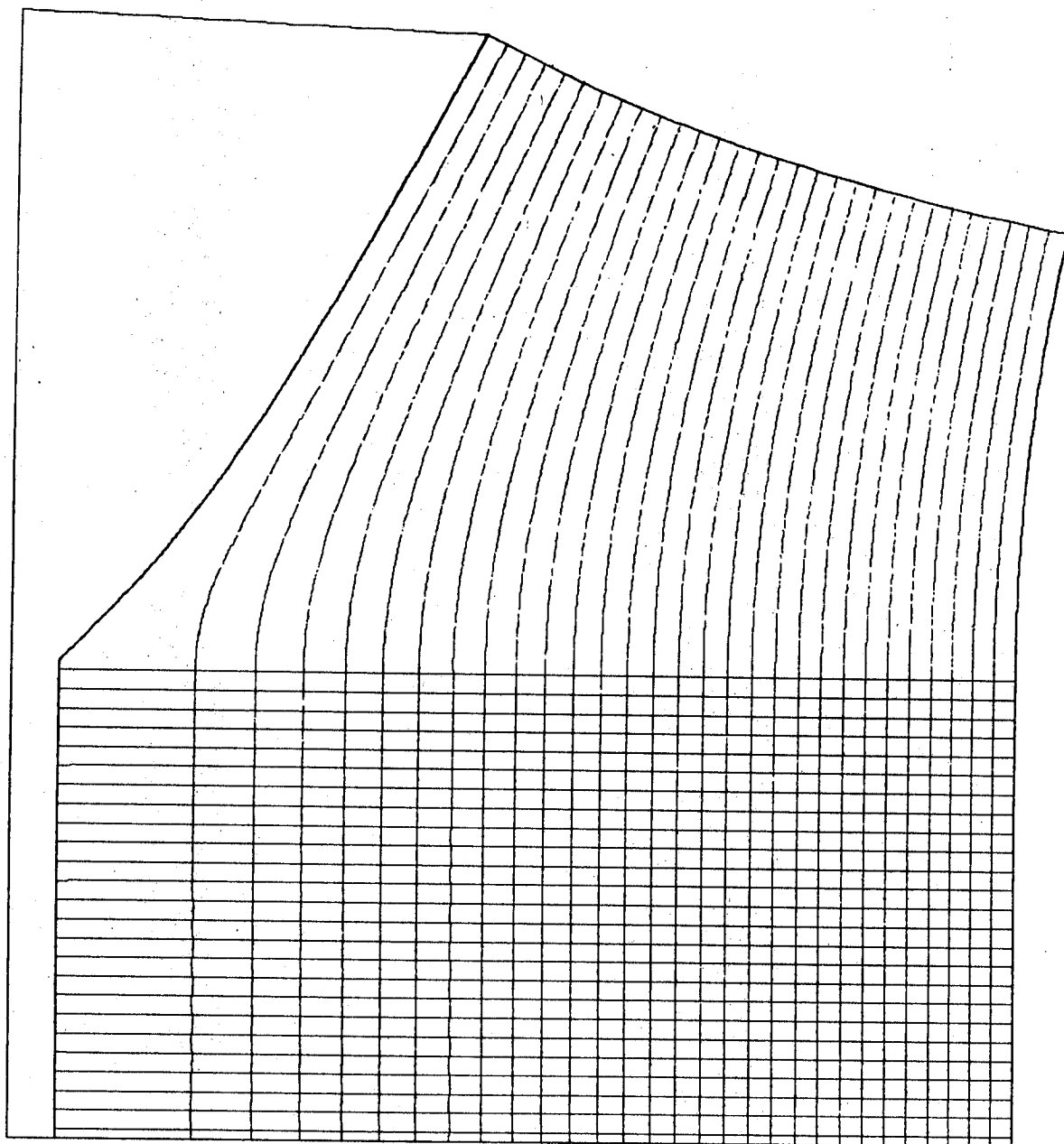Figure A5. Identification of quantities in a triangle.
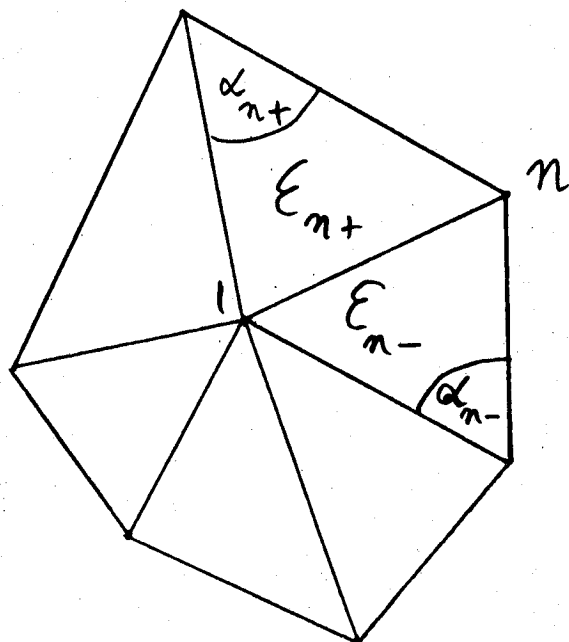
$A\ 6$

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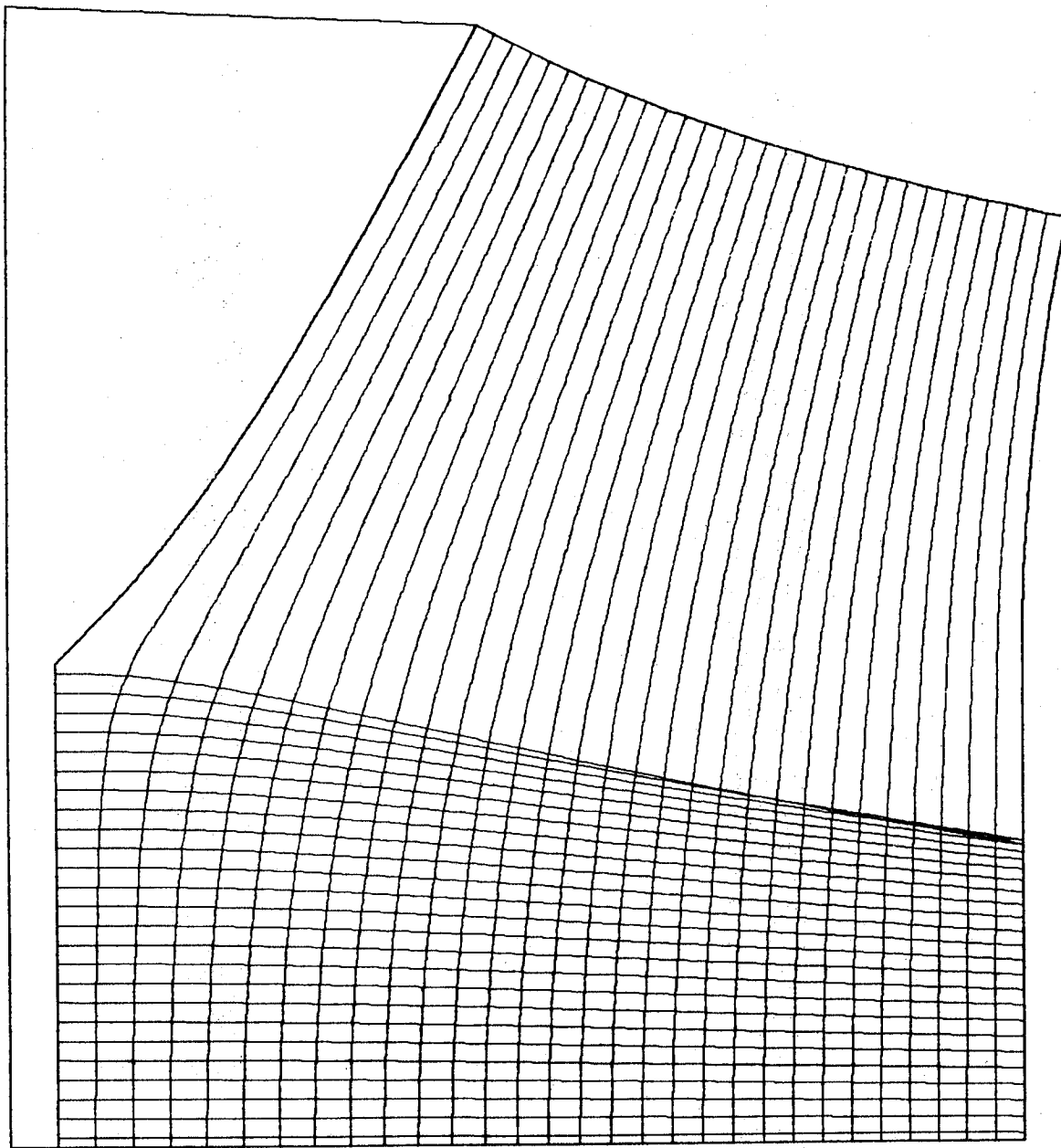Figure A6. Identification of quantities in a triangle.

$D\ 1$

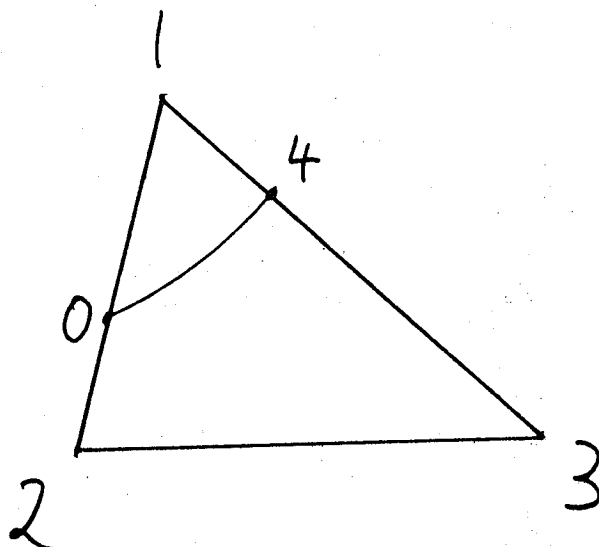Figure D1. Identification of X_R, X_L, and y_T, y_B.

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Figure F1. Initial equipotentials and ion trajectories in test problem.

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Figure F2. Final equipotentials and ion trajectories in test problem.

H1

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Figure H1.   Ion trajectory in triangle.